3-((E)-2-Methylbut-2-enamido)propyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C13H21NO3/c1-5-10(3)12(15)14-8-7-9-17-13(16)11(4)6-2/h5-6H,7-9H2,1-4H3,

InchiKey: SVVFURUTCNYAPB-YOYBCKCWSA-N

Formula: C13H21NO3

SMILES: CC=C(C)C(=O)NCCCOC(=O)C(C)=CC

Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
gf	-71.53	kJ/mol	Joback Method
hf	-400.70	kJ/mol	Joback Method
hfus	36.69	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.968		Crippen Method
mcvol	204.420	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
tb	685.25	K	Joback Method
tc	881.19	K	Joback Method
tf	372.94	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.95	J/mol×K	685.25	Joback Method
cpg	566.33	J/mol×K	717.91	Joback Method
cpg	579.92	J/mol×K	750.56	Joback Method
cpg	592.76	J/mol×K	783.22	Joback Method
cpg	604.89	J/mol×K	815.88	Joback Method
cpg	616.34	J/mol×K	848.53	Joback Method
cpg	627.16	J/mol×K	881.19	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume